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# Simulation of Aluminium Combustion and PETN Afterburning in a Confined Explosion

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## 1 Introduction

We investigate the combustion occurring in shock-dispersed-fuel (SDF) explosions in a calorimeter [1]. The SDF charge consisted of a 0.5-g spherical PETN ( $C_5H_8N_4O_{12}$ ) charge surrounded by 1 gram of fuel. Various fuels have been used, such as: flake Aluminum ( $Al$ ), ball-milled activated carbon ( $C_s$ ), polyethylene ( $CH_2-CH_2$ ) granules, sucrose ( $C_{12}H_{22}O_{11}$ ) powder and TNT ( $C_7H_5N_3O_6$ ). As the PETN detonation products expand, they disperse and heat the fuel; when the so-prepared fuel mixes with air, it releases its Heat of Combustion via turbulent combustion [2]. Such heats of combustion vary from  $\sim 3,500$  cal/g for TNT and 7,400 cal/g for  $Al$ , up to 10,500 cal/g for hydrocarbons. This raises the chamber temperature to 2,300–3,700 K (depending on the fuel) and induces a corresponding increase in chamber pressure. Described here are high-resolution numerical simulations of that confined turbulent combustion process.

In ICDERS-20, we presented numerical simulations of after-burning of TNT-SDF charge in a chamber. We also traced the solution in thermodynamic state space—thereby discovering the *combustion locus* that constrains the solution [3]. In the meantime, we have developed a two-phase Model [4] suitable for treating particle combustion in SDF explosions. It utilizes an equilibrium-chemistry approach [5] for the gas phase  $Al$  combustion with air (this allows us to focus computational power on the gasdynamics and turbulent mixing fields which control the process). Preliminary simulations of an  $Al$ -SDF explosion in a 6.6-liter calorimeter were presented at the 41<sup>st</sup> JANNAF Conference [6].

Presented here are high-resolution numerical simulations of  $Al$ -SDF explosions in various chambers, including the effects of after-burning of PETN detonation products gases with air (an effect neglected previously [6]). The two-phase Model is delineated in the next section. This is followed by results for 3-D simulations of  $Al$  combustion in explosions.

## 2 Model

We model evolution of the combustion field in the limit of large Reynolds and Peclet numbers, where molecular diffusion and heat conduction effects in the gas phase are negligible. The flow field is then governed by the gas-dynamic conservation laws:

$$\text{Mass:} \quad \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = \dot{\sigma}_s \quad (1)$$

$$\text{Momentum:} \quad \partial_t \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p) = \dot{\sigma}_s \mathbf{v} - \dot{f}_s \quad (2)$$

$$\text{Energy:} \quad \partial_t \rho E + \nabla \cdot (\rho \mathbf{u} E + p \mathbf{u}) = -\dot{q}_s + \dot{\sigma}_s E_s - \dot{f}_s \cdot \mathbf{v} \quad (3)$$

where  $\rho, p, \mathbf{u}$  represent the gas density, pressure and specific internal energy,  $\mathbf{u}$  is the gas velocity vector, and  $E \equiv u + \mathbf{u} \cdot \mathbf{u} / 2$  denotes the total energy of the gas phase. Source terms on the right hand side take into account: mass addition to gas phase due to particle burning ( $\dot{\sigma}_s$ ), particle drag ( $\dot{f}_s$ ), and heat losses ( $\dot{q}_s$ ).

We treat the particle phase as continuum. We consider the dilute limit, devoid of particle-particle interactions, so that the pressure and sound speed of the particle phase are zero. We model the evolution of particle phase mass, momentum and energy fields by the conservation laws of continuum mechanics for heterogeneous media as described by Nigmatulin [7]:

$$\text{Mass:} \quad \partial_t \sigma + \nabla \cdot \sigma \mathbf{v} = -\dot{\sigma}_s \quad (4)$$

$$\text{Momentum:} \quad \partial_t \sigma \mathbf{v} + \nabla \cdot \sigma \mathbf{v} \mathbf{v} = -\dot{\sigma}_s \mathbf{v} + \dot{f}_s \quad (5)$$

$$\text{Energy:} \quad \partial_t \sigma E_s + \nabla \cdot \sigma E_s \mathbf{v} = \dot{q}_s - \dot{\sigma}_s E_s + \dot{f}_s \cdot \mathbf{v} \quad (6)$$

$$\text{Number particles:} \quad \partial_t n_s + \nabla \cdot n_s \mathbf{v} = 0 \quad (7)$$

where  $\sigma$  and  $\mathbf{v}$  represent the particle-phase density and velocity while  $E_s \equiv C_s T_s + \mathbf{v} \cdot \mathbf{v} / 2$  denotes the total energy of the particle phase.

The inter-phase interaction terms for mass, momentum, heat and particle burning take the form [8]:

$$\text{Mass Exchange:} \quad \dot{\sigma}_s = \begin{cases} 0 & T_s < T_{ign} \\ -3\sigma(1 + 0.276\sqrt{\text{Re}_s})/t_s & T_s \geq T_{ign} \end{cases} \quad \text{where } t_s = Kd_{s0}^2 \text{ (see [9])} \quad (8)$$

$$\text{Momentum Exchange:} \quad \dot{f}_s = \frac{3}{4} \frac{\rho}{\rho_s} \frac{\sigma}{d_s} C_D (\mathbf{u} - \mathbf{v}) |\mathbf{u} - \mathbf{v}| \quad (9)$$

$$\text{where} \quad C_D = 24 / \text{Re}_s + 4.4 / \sqrt{\text{Re}_s} + 0.42 \quad \text{and} \quad \text{Re}_s = \rho d_s |\mathbf{u} - \mathbf{v}| / \mu \quad (10)$$

$$\text{Heat Exchange:} \quad \dot{q}_s = \frac{6\sigma}{\rho_s d_s} \left[ \frac{Nu\lambda(T - T_s)}{d_s} + \varepsilon \sigma_{\text{Boltz}} (T^4 - T_s^4) \right] \quad \text{where } Nu = 2 + 0.6 \text{Pr} \sqrt{\text{Re}_s} \quad (11)$$

We recognize two fuels: PETN detonation products ( $F_1$ ) and Aluminum ( $F_2$ ), along with their corresponding combustion products: PETN-air ( $P_1$ ) and Al-air ( $P_2$ ). We consider the global combustion of fuel  $F_k$  with air ( $A$ ) producing equilibrium combustion products  $P_k$ :  $F_k + A \Rightarrow P_k$  with  $k = 1$  or  $2$ . The mass fractions  $Y_k$  of the components are governed by the following conservation laws:

$$\text{Fuel-}k: \quad \partial_t \rho Y_{F_k} + \nabla \cdot \rho Y_{F_k} \mathbf{u} = -\dot{s}_k + \delta_{k2} \dot{\sigma}_k \quad (12)$$

$$\text{Air:} \quad \partial_t \rho Y_A + \nabla \cdot \rho Y_A \mathbf{u} = -\sum_k \alpha_k \dot{s}_k \quad (13)$$

$$\text{Products-}k: \quad \partial_t \rho Y_{P_k} + \nabla \cdot \rho Y_{P_k} \mathbf{u} = \sum_k (1 + \alpha_k) \dot{s}_k \quad (14)$$

In the above,  $\dot{s}_k$  represents the global kinetics source/sink term. In this work we use the fast-chemistry limit that is consistent with the inviscid gas-dynamic model (1)-(3), so whenever fuel and air enter a computational cell, they are consumed in stoichiometric proportions:  $\alpha_k = A / F_k$  during one time step. The symbol  $\delta_{k2}$  represents the Kronecker delta. To clarify the notation of (12)-(14), the case of  $k=1$  denotes PETN-air afterburning while

the case of  $k=2$  corresponds Al-air combustion. In addition, two global simultaneous combustion processes can also be considered (assuming that the fuels  $F_k$  do not react with each other). Combination  $k=\{1,2\}$  models the afterburning of PETN and combustion of Al with air in an Al-SDF explosion.

The thermodynamic states encountered during the combustion of the aluminum powder with air are depicted by the Le Chatelier diagram of Fig. 1. The Reactants-R are defined as a stoichiometric mixture of air and Aluminum in *frozen* composition (air/fuel ratio:  $\alpha_s = 4.03$ ). The Products-P are assumed to be in *thermodynamic equilibrium*. These states were calculated with the Cheetah code. These states have been fit with quadratic functions that then serve as analytic Equations of State [5].

### 3 Results

Numerical simulations of the explosion of a 1.5-g Al-SDF charge (0.5-g PETN booster + 1.0-g flake Al fuel) in a 6.6-liter calorimeter were performed with the two-phase Adaptive Mesh Refinement (AMR) code. A cross-sectional view of the combustion products field is presented in Fig. 2. Such visualizations illustrate that the flow field is turbulent.

Pressure histories are shown in Fig. 3. Pressures measured for an explosion in air (red curve) are much larger than pressures measured for an explosion in nitrogen (blue curve). This is due to thermo-baric effects, namely: combustion of the Al fuel with air and after-burning of the PETN detonation products with air. The black curve represents results from two-phase 3d AMR code for PETN/Al combustion in air. Computed waveforms are very similar to the experimental waveforms—thereby demonstrating that the two-phase AMR code can accurately predict the evolution of combustion fields in such explosions.

### 4 Conclusions

Numerical simulations of the combustion of Aluminum particles in shock-dispersed-fuel explosions have been presented. For the problem studied, two-phase effects are very important—especially during the initial expansion of the blast wave (i.e., during the particle dispersion phase of the problem). The two-phase model allows the PETN detonation products gases to slip through the fuel region, accelerating the particles and afterburning with air. This leads to heating the fuel and igniting the Al-air mixture to form a combustion cloud. Single-phase models do not capture these important physical effects. This is a non-premixed combustion problem, so the combustion rate is controlled by the mixing rate. By using adaptive mesh refinement, we are able to capture enough of the mixing scales to achieve physically realistic burning rates. This is confirmed by comparison of pressure histories in Fig. 3.

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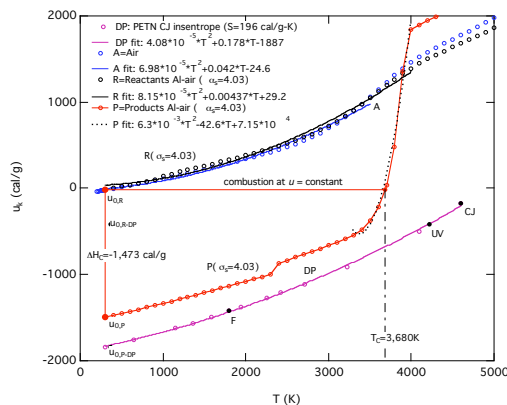


Figure 1. Le Chatelier diagram for stoichiometric combustion of aluminum in air ( $\alpha_s = 4.03$ ).

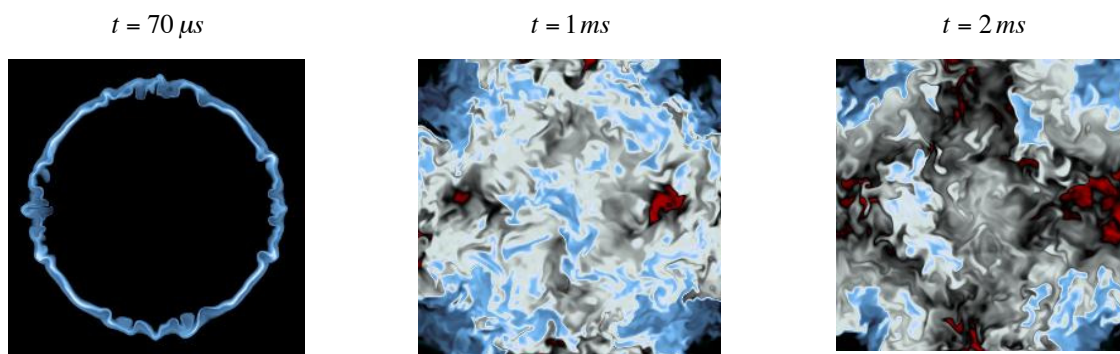


Figure 2. Cross-sectional view of the combustion Products field as predicted by the 3d-AMR simulation.

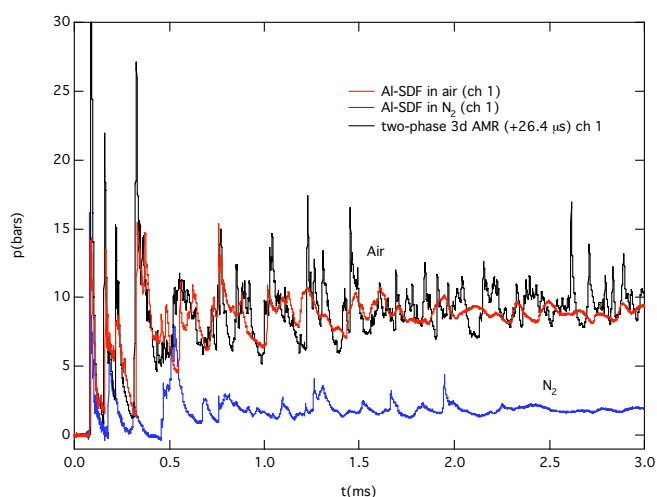


Figure 3. Pressure histories from an explosion of a 1.5-g Al-SDF charge in a 6.6-liter calorimeter.